

Flow Equations for the Ionic Hubbard Model

Mohsen Hafez,¹ S. A. Jafari*,^{2,3} and M. R. Abolhassani¹

¹*Department of Physics, Tarbiat Modares University, Tehran, Iran*

²*Department of Physics, Isfahan University of Technology, Isfahan 84154-83111, Iran*

³*The Abdus Salam ICTP, 34100 Trieste, Italy*

Taking the site-diagonal terms of the one-dimensional ionic Hubbard model (IHM) as H_0 , we employ Continuous Unitary Transformations (CUT) to obtain a "classical" effective Hamiltonian in which hopping term has been integrated out. For this Hamiltonian spin gap and charge gap are calculated at half-filling and subject to periodic boundary conditions. Our calculations indicate two transition points. In fixed Δ , as U increases from zero, there is a region in which both spin gap and charge gap are positive and identical; characteristic of band insulators. Upon further increasing U , first transition occurs at $U = U_{c1}$, where spin and charge gaps both vanish and remain zero up to $U = U_{c2}$. A gap-less state in charge and spin sectors characterizes a metal. For $U > U_{c2}$ spin gap remains zero and charge gap becomes positive. This third region corresponds to a Mott insulator in which charge excitations are gaped, while spin excitations remain gap-less.

PACS numbers: 71.10.Fd, 78.66.Nk, 77.22.Ej

INTRODUCTION

Ionic Hubbard model (IHM) has been used to study neutral-ionic transition in organic compounds [1] and understanding role of strong correlations in ferroelectricity of metal oxides such as BaTiO₃, KNbO₃, KTaO₃ [2], as well as some quasi one-dimensional materials such as (TaSe₄)₂I, K_{0.3}MoO₃ [3]. IHM Hamiltonian includes an staggered one-body external potential in addition to the Hubbard Hamiltonian. The Hamiltonian for this model is as follows:

$$H = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + U \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} + \frac{\Delta}{2} \sum_{i\sigma} (-1)^i c_{i\sigma}^\dagger c_{i\sigma}, \quad (1)$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the usual annihilation (creation) operator at site i with spin σ , t the nearest neighbor hopping amplitude, U the on-site coulomb interaction parameter, and Δ a one-body ionic potential. This model has a very interesting phase diagram at zero temperature at half-filling. When $\Delta \ll U$ this Hamiltonian, like the usual Hubbard Hamiltonian, is transformed to the Heisenberg spin Hamiltonian [1, 5] that describes a Mott insulator. In the opposite limit $\Delta \gg U$, one can ignore U , and a Bogoliubov transformation gives a simple band insulator with gap Δ . The limit $U \gg \Delta$ is a many-body insulator, while the limit $U \ll \Delta$ is a one-body insulator. Hence this model is a basis to study the issues like matrix-element effects in optical spectra of band insulators, versus many-body insulators [6].

Apart from offering two entirely different insulating states, yet there remains interesting question of the intermediate phase: What is the nature of the ground state for $U \sim \Delta$? Researchers have used various methods such as exact diagonalization (ED) [2, 4], density matrix renormalization group

(DMRG) [7, 8, 9], quantum Monte Carlo (QMC) [1, 10, 11, 12], dynamical mean field theory (DMFT) [13, 14, 15], etc. to study the properties of this model.

The nature of intermediate phase still remains controversial: Bosonization study of Fabrizio and coworkers [16] indicates an spontaneously dimerized phase, which is also supported by spin-particle transformation study of Batista and coworkers [17]. There are also other works supporting this scenario [7, 8, 11, 15]. On the other hand, there are studies showing that the intermediate phase is metallic [1, 4, 10, 13]. Brune finds a metallic transition point in between the band and Mott insulating states, with simultaneous bond order [9]. Craco et. al. in addition to metallic region, report on a coexistence phase between the band and Mott insulating states [14].

In this work, we employ the method of continuous unitary transformations or flow equations to study the half-filled one-dimensional IHM in zero temperature subject to periodic boundary conditions. CUT method is used to obtain a "classical" effective Hamiltonian for IHM. This effective Hamiltonian which is free of fermionic minus sign problem, provides a simple picture of the nature of excitations when interpreted in terms of the transformed ground state. Then for $L = 20$ sites and with $\Delta = 20$ (energies are in units of t) spin and charge gap are numerically calculated for different values of U . These calculations indicate two transition points. For $U < U_{c1}$, spin and charge gap are both positive, for $U_{c1} < U < U_{c2}$ are both zero and for $U > U_{c2}$ spin gap remains zero while charge gap becomes positive. Hence this the transformed effective Hamiltonian gives band insulator for small U region ($U < U_{c1}$), Mott insulator for large U regime ($U > U_{c2}$), and metal for the region in between.

ATOMIC LIMIT

In the limits $U \ll \Delta$ and $\Delta \ll U$, the model becomes easy to understand and gives band and Mott insulators, respectively. Yet, another interesting limit in which the phase dia-

*Electronic address: akbar.jafari@gmail.com

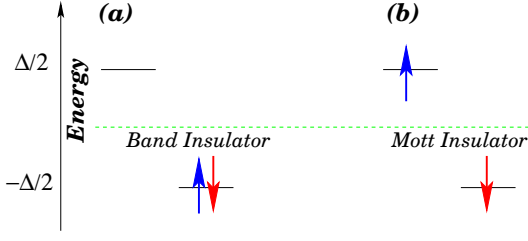


FIG. 1: (Color online) Lowest energy configurations for (a) Perfect band insulator, (b) Perfect Mott insulator.

gram becomes particularly simple is the atomic limit ($t = 0$),

$$E[n_{i\sigma}] = \frac{\Delta}{2} \sum_{i\sigma} (-1)^i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where the Hamiltonian can be written solely in terms of classical (commuting) variables $n_{i\sigma}$. In this sense, the atomic limit corresponds to the classic limit of a quantum problem, and it becomes much easier to analyze. Any configuration $\{|n_{i\sigma}\rangle\}$ is an eigen-state of this Hamiltonian. The hopping term which causes quantum fluctuations of various $\{|n_{i\sigma}\rangle\}$ configurations by admixing them is absent here. Hence the problem reduces to finding out the configuration with lowest energy. To this end, we consider a unit cell in real space of the 1D lattice shown in Fig. 1. Since this Hamiltonian contains purely local degrees of freedom, we consider a zero momentum mode ($k = 0$) which corresponds to repeating this unit cell all over the 1D chain. In part (a), a state with energy $E_a = U - \Delta$ per unit cell is shown, while the one in part (b) has energy $E_b = 0$ per unit cell. For $E_a < E_b$, i.e. $U - \Delta < 0$, state (a) indicating a band insulator is stabilized, while for $U > \Delta$, the Mott insulating state with energy E_b is stabilized. At $U = \Delta$ these two states are degenerate, and hence in $k = 0$ mode, \uparrow spin can freely move in the unit cell of Fig. 1. Therefore the picture in the atomic limit is as follows: Eq. (2) describes a Mott insulator for $\Delta < U$ and a band insulator for $\Delta > U$. The transition line $\Delta = U$ is a metal phase shrunk to a line.

The question we would like to address in this paper is, what happens if we turn on the quantum fluctuations around the Hamiltonian (2) by introducing a finite hopping t ? It turns out that CUT is a very suitable tool to investigate this *strong coupling* problem. We advertise the result in advance: The inclusion of the hopping t will renormalize $U \rightarrow \tilde{U}(t, U, \Delta)$, $\Delta \rightarrow \tilde{\Delta}(t, U, \Delta)$, $t \rightarrow \tilde{t} = 0$, as well as generating new couplings.

CONTINUOUS UNITARY TRANSFORMATIONS

Flow equations approach or, CUT method [18] was introduced independently by Glazek and Wilson [19], and Wegner [20]. Since then, this method has been applied extensively to study various models in condensed matter and high energy physics. Some examples include, the Anderson model [21],

Lipkin model [22], mapping of the electron-phonon interaction to an effective electron-electron interaction [23], Sine-Gordon model [24], RKKY interaction [25], as well as non-equilibrium dynamics of strongly correlated systems [26] and an attempt for a unified description of Fermi and Luttinger liquids in all energy scales [27].

In this method the Hamiltonian is transformed by a unitary operator $U(\ell)$ where ℓ is a parameter between zero to infinity. Flow equation for $H(\ell) = U^\dagger(\ell) H U(\ell)$ becomes,

$$\partial_\ell H(\ell) = [\eta(\ell), H(\ell)], \quad (3)$$

where $\eta(\ell) = \partial_\ell U^\dagger(\ell) U(\ell)$ is an anti-Hermitian operator called generator. Here $U(\ell = 0) = 1$, as at $\ell = 0$ transformed Hamiltonian is equal to H . Wegner suggested the following generator [20]:

$$\eta(\ell) = [H^d(\ell), H^r(\ell)], \quad (4)$$

where $H^d(\ell)$ ($H^r(\ell)$) is diagonal (off-diagonal) part of the Hamiltonian. With this choice for the generator, transformed Hamiltonian flows towards a diagonal or block-diagonal form in the $\ell \rightarrow \infty$ limit. Mielke introduced another generator that is specially useful for band matrices [28] and preserves the band nature of the Hamiltonian matrix. In this section, we use Wegner generator to obtain an effective Hamiltonian for IHM.

It is obvious from Eq. (3) that the flow equations without any approximation is very hard to solve for Hamiltonians that include interaction. In applying the flow equations to IHM we use an approximation similar to the one used by Kehrein and Mielke in the context of Anderson model [21]. We approximate $H(\ell)$ as,

$$\begin{aligned} H(\ell) = & -t(\ell) \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + \frac{\Delta(\ell)}{2} \sum_{i\sigma} (-1)^i c_{i\sigma}^\dagger c_{i\sigma} \\ & + \frac{U(\ell)}{2} \sum_{i\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} \\ & + V(\ell) \sum_{i\sigma\sigma'} c_{i\sigma}^\dagger c_{i+1\sigma'}^\dagger c_{i+1\sigma'} c_{i\sigma}. \end{aligned} \quad (5)$$

with initial conditions $t(0) = 1$, $\Delta(0) = \Delta$, $U(0) = U$ and $V(0) = 0$. Physical motivation behind considering n.n. Coulomb interaction V is as follows [8]: In the simple phase diagram shown in Fig. 1 for a fixed Δ , as one increases U , the ionicity $n_B - n_A$ which is the population difference between A, B lattice sites, suddenly drops from 1 to 0 at $U_{c2} = \Delta$. If an attractive n.n. term V can be generated, it opens up an intermediate phase in which the $0 < n_B - n_A < 1$; i.e. the unit cell gently loses its polarization with respect to the half-filled background and turns into a Mott insulator.

In Eq. (5), the first term is taken to be off diagonal and other terms are diagonal. This choice resembles the strong coupling perturbation schemes starting from the atomic limit. There one usually has to organize the hopping processes into those terms which change the double occupancy, and those which do not [5]. But here we show that the inclusion of smallest

amount of Δ makes it possible to renormalize the whole hopping processes to zero (Eq. 14).

Using equation (4), With this convention, the Wegner generator is obtained as:

$$\begin{aligned} \eta(\ell) = & t(\ell)\Delta(\ell) \sum_{i\sigma} (-1)^i (c_{i+1\sigma}^\dagger c_{i\sigma} - h.c.) \\ & - t(\ell)U(\ell) \sum_{i\sigma\sigma'} (c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i+1\sigma} - c_{i-1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} - h.c.) \\ & - t(\ell)V(\ell) \sum_{i\sigma\sigma'} (c_{i\sigma}^\dagger c_{i+1\sigma'}^\dagger c_{i+1\sigma'} c_{i+1\sigma} + c_{i\sigma}^\dagger c_{i+1\sigma'}^\dagger c_{i+2\sigma'} c_{i\sigma} \\ & - c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i+1\sigma'} c_{i\sigma} - c_{i-1\sigma}^\dagger c_{i+1\sigma'}^\dagger c_{i+1\sigma'} c_{i\sigma} - h.c.) \end{aligned} \quad (6)$$

To obtain the flow equations, we need to calculate the commutator of $\eta(\ell)$ and $H(\ell)$. To do so, we split $\eta(\ell)$ into three parts

$$\eta(\ell) = \eta_1(\ell) + \eta_2(\ell) + \eta_3(\ell), \quad (7)$$

where $\eta_1(\ell)$, $\eta_2(\ell)$, and $\eta_3(\ell)$ denote the first, second, and third terms in equation (6) respectively. Similarly, $H(\ell)$ in equation (5) has four terms

$$H(\ell) = H_1(\ell) + H_2(\ell) + H_3(\ell) + H_4(\ell), \quad (8)$$

where $H_1(\ell) \dots H_4(\ell)$ correspond to four terms in Eq. (5). Therefore:

$$\begin{aligned} [\eta(\ell), H(\ell)] = & [\eta_1(\ell), H_1(\ell) + H_2(\ell)] + [\eta_2(\ell), H_1(\ell)] \\ & + [\eta_3(\ell), H_1(\ell)] + \text{irrelevant terms}, \end{aligned} \quad (9)$$

where "irrelevant terms" are newly generated couplings which are not similar to Eq. (5). The commutators are calculated as follows:

$$\begin{aligned} [\eta(\ell), H_1(\ell) + H_2(\ell)] = & 2t^2(\ell)\Delta(\ell) \sum_{i\sigma} (-1)^i (c_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{i+2\sigma} + h.c.) \\ & + t(\ell)\Delta^2(\ell) \sum_{i\sigma} (c_{i+1\sigma}^\dagger c_{i\sigma} + h.c.), \end{aligned} \quad (10)$$

and

$$\begin{aligned} [\eta_2(\ell), H_1(\ell)] = & t^2(\ell)U(\ell) \sum_{i\sigma\sigma'} \sum_{j\beta} \times \\ & ([c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i+1\sigma}, c_{j\beta}^\dagger c_{j+1\beta}] + [c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i+1\sigma}, c_{j+1\beta}^\dagger c_{j\beta}] \\ & - [c_{i-1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma}, c_{j\beta}^\dagger c_{j+1\beta}] - [c_{i-1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma}, c_{j+1\beta}^\dagger c_{j\beta}] \\ & + h.c.). \end{aligned} \quad (11)$$

First and third terms are irrelevant, while second and fourth terms respectively become

$$\begin{aligned} & (c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} \delta_{i,j} \delta_{\sigma\beta} - c_{i+1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i+1\sigma} \delta_{i,j} \delta_{\sigma\beta}) - \\ & (c_{i-1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i-1\sigma} \delta_{i,j+1} \delta_{\sigma\beta} - c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} \delta_{i-1,j} \delta_{\sigma\beta}) \\ & + \text{irrelevant terms}. \end{aligned}$$

Substituting in Eq. (11) and dropping irrelevant terms gives,

$$\begin{aligned} [\eta_2(\ell), H_1(\ell)] = & 2t^2(\ell)U(\ell) \\ & \times \sum_{i\sigma\sigma'} (c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} - c_{i+1\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i+1\sigma} + h.c.) \end{aligned} \quad (12)$$

The last commutator up to irrelevant terms becomes:

$$\begin{aligned} [\eta_3(\ell), H_1(\ell)] = & 2t^2(\ell)V(\ell) \\ & \times \sum_{i\sigma\sigma'} (2c_{i\sigma}^\dagger c_{i+1\sigma'}^\dagger c_{i+1\sigma'} c_{i\sigma} - c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} + h.c.) \end{aligned} \quad (13)$$

Substitution of Eqs. (10), (12) and (13) in Eq. (9), gives the following set of flow equations

$$\partial_\ell t(\ell) = -t(\ell)\Delta^2(\ell) \quad (14)$$

$$\partial_\ell \Delta(\ell) = 8t^2(\ell)\Delta(\ell) \quad (15)$$

$$\partial_\ell U(\ell) = 8t^2(\ell)(U(\ell) - V(\ell)) \quad (16)$$

$$\partial_\ell V(\ell) = 4t^2(\ell)(2V(\ell) - U(\ell)) \quad (17)$$

We obtain a closed form solution for the above set of equations at $\ell \rightarrow \infty$.

$$t(\infty) = 0 \quad (18)$$

$$\Delta(\infty) = (8 + \Delta^2)^{\frac{1}{2}} \quad (19)$$

$$U(\infty) = \frac{U}{2} \frac{(8 + \Delta^2)^{\frac{1}{2}} ((8 + \Delta^2)^{\frac{\sqrt{2}}{4}} + (8 + \Delta^2)^{\frac{-\sqrt{2}}{4}} \Delta^{\sqrt{2}})}{\Delta^{1 + \frac{\sqrt{2}}{2}}} \quad (20)$$

$$V(\infty) = \frac{\sqrt{2}U}{4} \frac{(8 + \Delta^2)^{\frac{1}{2}} ((8 + \Delta^2)^{\frac{\sqrt{2}}{4}} + (8 + \Delta^2)^{\frac{-\sqrt{2}}{4}} \Delta^{\sqrt{2}})}{\Delta^{1 + \frac{\sqrt{2}}{2}}} \quad (21)$$

Eq. (18) shows that the Hamiltonian is diagonal in infinity. The hopping term has been renormalized to zero. This has become possible because of the existence of a non-zero value of $\Delta(\ell = 0)$ (Eq. 14). Presence of any non-zero Δ changes the symmetry of the problem, and also introduces a new energy scales which makes the life different from that of the usual Mott-Hubbard physics. In case of a pure Hubbard model, one needs to take split the hopping terms into those which change the double occupancy, and those which do not [30, 31]. But here due to presence of a new energy scale, Δ , the whole hopping term can be renormalized to zero.

Eqs. (19), (20), and (21) indicate that the result of integrating out the hopping term in the Hamiltonian renormalizes the diagonal terms. Integrating out the hopping term also induces new coupling which are not of the form (5), and hence irrelevant. Therefore the fixed point of the one dimensional IHM is described by the effective Hamiltonian

$$\begin{aligned} H(\infty) = & \frac{\Delta(\infty)}{2} \sum_{i\sigma} (-1)^i n_{i\sigma} + U(\infty) \sum_i n_{i\uparrow} n_{i\downarrow} \\ & + V(\infty) \sum_{i\sigma\sigma'} n_{i\sigma} n_{i+1\sigma'}, \end{aligned} \quad (22)$$

where $n_{i\sigma}$ is the number of electron in site i with spin σ . Also note from Eq. (21) that for any $U, \Delta > 0$, $V(\infty)$ is always negative. Hence the induced n.n. Coulomb interaction is attractive. As a consistency check we note that our effective Hamiltonian in the limit $U, \Delta \gg 1$ Eq. (22) reduces to the atomic limit ($t = 0$) of Eq. (1).

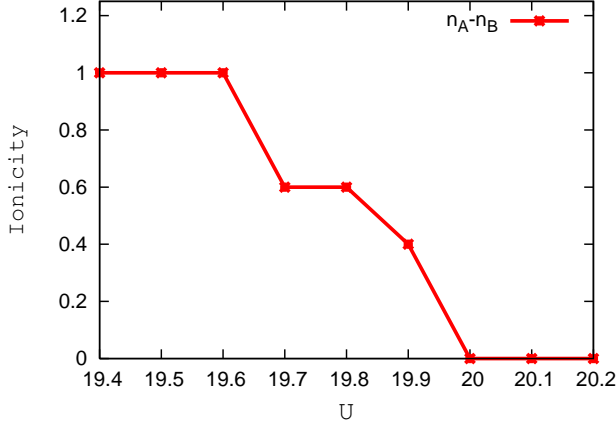


FIG. 2: Ionicity for $\Delta = 20$, $t = 1$ and $L = 20$ sites.

PHASE TRANSITIONS

Ionicity

Fig. 1 represents two limiting case of the Hamiltonian (2). For the band insulator, where both electrons of spin \uparrow and \downarrow prefer the B sites with energy $-\Delta/2$, the unit cell is fully polarized. In the opposite limit of the Mott insulator, there is only one electron per site, and the unit cell polarization is zero. Therefore we define the ionicity for IHM as $n_B - n_A$ where n_B and n_A are the density of electron in B and A sites respectively:

$$n_B = \frac{1}{N} \sum_{\sigma, i \in B} \langle \hat{n}_{i\sigma} \rangle \quad (23)$$

$$n_A = \frac{1}{N} \sum_{\sigma, i \in A} \langle \hat{n}_{i\sigma} \rangle \quad (24)$$

The ionicity for the IHM is depicted in Fig. 2. As can be seen in the figure, the ionicity is 1 for $U < U_{c1}$, indicating a band insulating state. For $U > U_{c2}$, the ionicity becomes zero, characterizing a Mott insulator. The intermediate region $U_{c1} < U < U_{c2}$ is characterized by $1 > n_B - n_A > 0$. This basic physics is contained in *attractive* nature of the induced V term in Eq. (22). Without this term, there is only one phase transition at $U_c = \Delta$ (Eq. 2). However, the renormalization process leading to generation of V term, opens up an intermediate state allowing for the smooth decrease of the ionicity from 1 (Band insulator) to 0 (Mott insulator), by partially polarizing the unit cell.

In this picture the reduction in the degree of polarization of the unit cell to intermediate values facilitates the charge transfer between the two sites of each unit cell. Therefore the resulting intermediate state must be a metal.

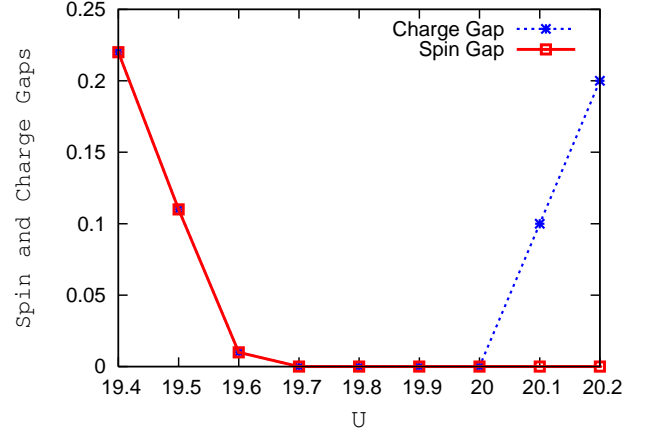


FIG. 3: Spin and charge gaps versus U for $\Delta = 20$, $t = 1$ and $L = 20$ sites.

Spin and charge gaps

To investigate the intermediate state further, we numerically calculate the charge and spin gaps for the IHM. Spin and charge gaps are defined as follows [29]

$$\Delta_s = E_0\left(\frac{N}{2} + 1, \frac{N}{2} - 1\right) - E_0\left(\frac{N}{2}, \frac{N}{2}\right), \quad (25)$$

$$\Delta_c = \frac{E_0\left(\frac{N}{2} + 1, \frac{N}{2} + 1\right) + E_0\left(\frac{N}{2} - 1, \frac{N}{2} - 1\right)}{2} - E_0\left(\frac{N}{2}, \frac{N}{2}\right), \quad (26)$$

where $E_0(N_\uparrow, N_\downarrow)$ is the ground state energy in a sector with N_\uparrow (N_\downarrow) electron in spin up (down) state. Since the unitary transformations do not affect the level spacing, the spin and charge gaps defined above will be the same for effective Hamiltonian (22) as well as the original Hamiltonian (1). Fortunately the effective Hamiltonian (22) is classical and hence free of fermionic minus sign issues. Therefore the ground state energy $E_0(N_\uparrow, N_\downarrow)$ in each sector can be numerically calculated with straight forward algorithms.

In Fig. 3 we have plotted the spin and charge gaps versus U for a fixed value of $\Delta = 20$. The numerical calculation is done for $L = 20$ lattice sites, subject to periodic boundary conditions. This figure shows two transition points at $U_{c1} = 19.7$ and $U_{c2} = 20$. For $U < U_{c1}$ spin and charge gap are positive and identical. The gaped charge excitations characterizes an insulating state. However, since the spin gap coincides with the charge gap, the resulting insulating state must be a simple band insulator. For $U_{c1} < U < U_{c2}$ spin and charge gap are both zero, characteristic of metallic states [4, 10, 13, 14].

Finally, for $U > U_{c2}$ charge excitations will become gaped, while spin excitations remain gap-less. Low-energy spin excitations, with gaped charge excitation is characteristic of Mott insulators. This picture is in agreement with the one emerging from Fig. 2, according to which, $n_i \equiv \sum_{\sigma} n_{i\sigma} = 1$.

For $\Delta = 1$ the transition points occur in $U_{c1} = 0.3$ and $U_{c2} = 0.7$ and for $\Delta = 2$ in $U_{c1} = 0.9$ and $U_{c2} = 1.7$. The phase diagram depicting the intermediate metallic region is shown in Fig. 4. In absence of t term, the metallic region

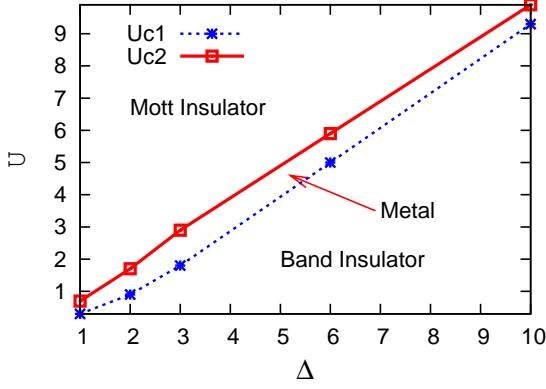


FIG. 4: Phase diagram of the IHM base on the effective Hamiltonian.

is characterized by line $U = \Delta$. In this case both U_{c1} and U_{c2} coincide and the metallic region shrinks to a line. However, inclusion of quantum fluctuations via t term, induces an attractive V term which eventually broadens the metallic line $U = \Delta$ into the narrow region shown in Fig. 4. In the limit $U, \Delta \gg t$ where the effective Hamiltonian reduces to the atomic limit (2), the intermediate region for a fixed Δ shrinks to zero and the metallic remains single point at $U_c = \Delta$ [10]. Therefore the large $\Delta, U \gg t$ limit of the Fig. 4 is a line on which band insulating and Mott insulating phases are degenerate.

In the ground state $|\tilde{\Psi}_0\rangle = |\Psi_0(\infty)\rangle$ of (22), the quantum fluctuations are frozen. The ground state of the original fermions is given by $|\Psi_0\rangle = \hat{U}(\infty)|\tilde{\Psi}_0\rangle$. When this transformation is applied, it is expected to restore the low-energy spin spectrum of the Mott insulating state, as well as the excitation spectrum of the resulting metallic state.

The question of whether the intermediate metallic state is a Fermi liquid, or non-Fermi liquid can be investigated by studying the dynamic correlation functions $\langle \Psi_0 | O_j(t) O_0(0) | \Psi_0 \rangle$. But since it is difficult to calculate $|\Psi_0\rangle$ of the original fermions, one can use the generator to set up flow equations for the observable \hat{O} , to calculate instead the quantity $\langle \tilde{\Psi}_0 | \tilde{O}_j(t) \tilde{O}_0(0) | \tilde{\Psi}_0 \rangle$. As far as the calculation of static quantities such as various energy gaps presented in this paper is concerned, the way one does the unitary transformation will not be important. But for dynamic correlation functions in order to capture the incoherent features in the electronic structure of strongly correlated systems such as IHM, one needs to organize the hopping processes depending on whether they change the double occupancy or not [30, 31].

To summarize, we have presented a strong coupling treatment of the ionic Hubbard model within the CUT approach. This enabled us to map the IHM into an effective Hamiltonian containing only commuting variables $n_{i\sigma}$. Getting rid of fermionic minus sign problems in this way, enables us to investigate the energetics of the model Hamiltonian, suggesting the phase diagram presented in Fig. 4.

ACKNOWLEDGEMENT

This work was partially supported by ALAVI Group Ltd. We would like to thank S. Kehrein, F. Shahbazi, M. Moeckel, P. Fritsch, for useful discussions. S.A.J. thanks S. Kehrein for hospitality during his visit to LMU, Munich.

-
- [1] N. Nagaosa and J. Takimoto, J. Phys. Soc. Jpn. **55**, 2735 (1986).
 - [2] T. Egami, S. Ishihara, and M. Tachiki, Science. **261**, 1307 (1993).
 - [3] M. C. Refolio, J. M. Lopez Sancho, and J. Rubio, J. Phys. Condens. Matter, **17**, 6635 (2005).
 - [4] N. Gidopoulos, S. Sorella, E. Tosatti, E. Phys. J. B **14**, 217 (2000).
 - [5] P. Fazekas, *Lecture notes on electron correlation and Magnetism*, World scientific, 1999
 - [6] T. Tohyama, S. Maekawa, J. Luminescence, **94-95**, 659 (2001).
 - [7] S. R. Manmana, V. Meden, R. M. Noack, and K. Schönhammer, Phys. Rev. B **70**, 155115 (2004).
 - [8] Ö. Legeza, K. Buchta, and J. Sólyom, Phys. Rev. B **73**, 165124 (2006).
 - [9] Ph. Brune, G. I. Japaridze, A. P. Kampf, and M. Sekania, cond-mat/0106007.
 - [10] K. Bouadim, N. Paris, F. Hébert, G. G. Batrouni, and R.T. Scalettar, Phys. Rev. B **76**, 085112 (2007); N. Paris, K. Bouadim, F. Hébert, G. G. Batrouni, and R. T. Scalettar, Phys. Rev. Lett. **98**, 046403 (2007).
 - [11] T. Wilkens and R.M. Martin, Phys. Rev. B **63**, 235108 (2001).
 - [12] M. C. Refolio, J. M. Lopez Sancho, and J. Rubio, cond-mat/0210462.
 - [13] A. Garg, H. R. Krishnamurthy, and M. Randeria, phys. Rev. Lett. **97**, 046403 (2006).
 - [14] L. Craco, P. Lombardo, R. Hayn, G.I. Japaridze, and E. Muller-Hartmann, cond-mat/0703814v2 (2007).
 - [15] S. S. Kancharla and E. Dagotto, Phys. Rev. Lett. **98**, 016402 (2007).
 - [16] M. Fabrizio, A. O. Gogolin and A. A. Nersesyan, Phys. Rev. Lett. **83**, 2014 (1999).
 - [17] C. D. Batista and A. A. Aligia, Phys. Rev. Lett. **92**, 246405 (2004).
 - [18] S. Kehrein, *The Flow Equation Approach to Many-Particle Systems*, Springer, 2006.
 - [19] S. D. Glazek and K. G. Wilson, Phys. Rev. D **48**, 5863 (1993).
 - [20] F. Wegner, Ann. Phys. (Leipzig) **3**, 77 (1994); F. Wegner, J. Phys. A: Math. Gen. **39**, 8221 (2006).
 - [21] S. Kehrein and A. Mielke, J. Phys. A **27**, 4259 (1994).
 - [22] J. Stein, J. Phys. G **26**, 377 (2000).
 - [23] P. Lenz and F. Wegner, Nucl. Phys. B **482**, 693 (1996).
 - [24] S. Kehrein, Phys. Rev. Lett. **83**, 4914 (1999).
 - [25] J. Stein, Eur. Phys. J. B **12**, 5 (1999).
 - [26] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008).
 - [27] C. P. Heidbrink, G. S. Uhrig, Phys. Rev. Lett. **88**, 146401 (2002).
 - [28] A. Mielke, Eur. Phys. J. B **5**, 605 (1998).
 - [29] C. Dziurzik, G. I. Japaridze, A. Schadschneider, and J. Zittartz, Eur. Phys. J. B **37**, 453463 (2004).
 - [30] A. Reischl, E. Muller-Hartmann, G. S. Uhrig, Phys. Rev. B **70**, 245124 (2004).

[31] S. Kehrein, private communication